

1,3-diphenylpropane-1,2-diol
5381-84-0 | DTXSID50281584

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.10e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.07e-01

Confidence level: 5.55e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4-(4-Hydroxy-4-methylpentyl)cyclohex-3-ene-1-carbaldehyde</div> <div>Measured: 2.90e-02</div> <div>Predicted: 1.89e-02</div>	<div>Image not found</div> <div>Terpin</div> <div>Measured: 2.06e-02</div> <div>Predicted: 3.89e-02</div>	<div>Image not found</div> <div>Terpin</div> <div>Measured: 2.06e-02</div> <div>Predicted: 3.89e-02</div>
<div>Image not found</div> <div>Nandrolone</div> <div>Measured: 1.13e-02</div> <div>Predicted: 3.08e-03</div>		